Two-dimensional few electron systems in high magnetic fields: Composite-fermion or rotating-electron-molecule approach?

Constantine Yannouleas and Uzi Landman
School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332-0430
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A new class of analytic and parameter-free, strongly correlated wave functions of simple functional form is derived for few electrons in two-dimensional quantum dots under high magnetic fields. These wave functions are constructed through breaking and subsequent restoration of the circular symmetry, and they offer a natural alternative to the Laughlin and composite-fermion functions. Underlying our approach is a collectively-rotating-electron-molecule picture. The angular momenta allowed by molecular symmetry correspond to the filling-factors' hierarchy of the fractional quantum Hall effect.

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Two-dimensional (2D) N-electron systems in strong magnetic fields have been the focus of extensive theoretical investigations in the last twenty years [1–13]. The reasons are twofold: (I) The early realization [1,2] that few electron systems are relevant to the physics of the fractional quantum Hall effect (FQHE) observed in the infinite 2D electron gas, and (II) The recent progress in nanofabrication techniques that has allowed experiments on 2D circular quantum dots (QD's) containing a finite number of electrons [14,15].

Among the many theoretical methods for studying such systems, two approaches have become well established, i.e., exact diagonalization techniques [1,4,8–10] and consideration of appropriate classes of strongly correlated, analytic trial wave functions in the complex plane [2–4]. The trial wave functions proposed todate have been based on physical intuition, and their justification has been inferred *a posteriori* through comparisons with exact numerical calculations and/or with the phenomenology of the FQHE.

In this paper, we use a systematic, *microscopic* approach and derive a *new class* of strongly correlated, analytic wave functions for the N-electron problem in strong magnetic fields [16]. Our analytic wave functions have a simple functional form which differs from that of the familiar composite-fermion (CF) [3] and Jastrow-Laughlin (JL) [2] functions, and they are associated with a physical picture of a collectively rotating electron molecule (REM). Guiding the synthesis of the states of the system, our approach consists of two steps: First the breaking of the rotational symmetry at the single-determinantal *unrestricted* Hartree-Fock (UHF) level yields states representing electron molecules (EM's, or finite crystallites). Subsequently the rotation of the electron molecule is described through restoration of the circular symmetry via post Hartree-Fock methods, and in particular Projection Techniques (PT's) [20]. Naturally, the restoration of symmetry goes beyond the mean-field and yields multideterminantal wave functions. Earlier we demonstrated that this method (generalized to include in addition the breaking of the total-spin symmetry) can describe accurately two-electron systems in molecular [17] and single [18] QD's at zero magnetic field [19].

In general, the symmetry-broken UHF [21] orbitals need to be determined numerically [12,13,17,18,22]. However, in the case of an infinite 2D electron gas in strong magnetic fields, it has been found [23] that such UHF orbitals [24] can be approximated by analytic Gaussian functions centered at different positions $Z_j \equiv X_j + \imath Y_j$ and forming an hexagonal Wigner crystal (each Gaussian representing a localized electron). The specific expression for these displaced Gaussians is

$$u(z, Z_j) = (1/\sqrt{\pi}) \times \exp[-|z - Z_j|^2/2] \exp[-\imath(xY_j + yX_j)] \ , \qquad (1)$$

where the phase factor is due to the gauge invariance. $z \equiv x - \imath y$, and all lengths are in dimensionless units of $l_B\sqrt{2}$ with the magnetic length being $l_B = \sqrt{\hbar c/eB}$.

In the case of a Coulombic finite N-electron system, it has been found [11,12] that the UHF orbitals arrange in concentric rings forming EM's (referred to also as Wigner molecules, WM's) [25]. The UHF results for the formation of WM's are in agreement with the molecular structures obtained via the conditional probability distributions (CPD's) which can be extracted from exact numerical wave functions [9,10,26]. For $N \leq 4$, the electrons are located at the apexes of a regular polygon situated on a single ring, while for $5 \leq N \leq 7$ both the single-ring structure and an isomeric one with one electron at the center come into play. We will denote the former arrangement as $(0, N)$ and the latter as $(1, N-1)$. The electrons of the $(0, N)$ ring are located at

$$Z_j = Z \exp[\imath 2\pi(1-j)/N], \ \ 1 \leq j \leq N \ , \qquad (2)$$

and those participating in a $(1, N-1)$ arrangement are located at

$$Z_1 = 0; \ Z_j = Z \exp[\imath 2\pi(2-j)/(N-1)], \ \ 2 \leq j \leq N \ . \qquad (3)$$

Before proceeding further, we need to expand the displaced Gaussian (1) over the Darwin-Fock single-particle

states. Due to the high magnetic field, only the single-particle states,

$$\psi_l(z) = \frac{z^l}{\sqrt{\pi l!}} \exp(-zz^*/2) \ , \tag{4}$$

of the lowest Landau level (LLL) are needed (observe that the angular momentum of this state is $-l$ due to the definition $z \equiv x - \imath y$). Then a straightforward calculation [27] yields

$$u(z,Z) = \sum_{l=0}^{\infty} C_l(Z)\psi_l(z) \ , \tag{5}$$

with $C_l(Z) = (Z^*)^l \exp(-ZZ^*/2)/\sqrt{l!}$ for $Z \neq 0$. Naturally, $C_0(0) = 1$ and $C_{l>0}(0) = 0$.

Since electrons in strong magnetic fields are fully polarized, only the space part of the many-body wave functions needs to be considered; for the symmetry-broken UHF determinant describing the WM, it is given by

$$\Psi^N_{\rm UHF} = \det[u(z_1,Z_1), u(z_2,Z_2), \cdots, u(z_N,Z_N)] \ . \tag{6}$$

Using (5) one finds the following expansion (within a proportionality constant)

$$\Psi^N_{\rm UHF} = \sum_{l_1=0,\ldots,l_N=0}^{\infty} \frac{C_{l_1}(Z_1)C_{l_2}(Z_2)\cdots C_{l_N}(Z_N)}{\sqrt{l_1!l_2!\cdots l_N!}} \times D(l_1,l_2,...,l_N) \exp(-\sum_{i=1}^{N} z_i z_i^*/2) \ , \tag{7}$$

where $D(l_1,l_2,...,l_N) \equiv \det[z_1^{l_1}, z_2^{l_2}, \cdots, z_N^{l_N}]$.

The UHF determinant [Eq. (6) or Eq. (7)] breaks the rotational symmetry and thus it is is not an eigenstate of the total angular momentum $\hbar\hat{L} = \hbar\sum_{i=1}^{N} \hat{l}_i$. However, one can *restore* the rotational symmetry by applying onto the UHF determinant the following projection operator [18,20]

$$2\pi\mathcal{P}_L \equiv \int_0^{2\pi} d\gamma \exp[i\gamma(\hat{L} - L)] \ , \tag{8}$$

where $\hbar L = \hbar\sum_{i=1}^{N} l_i$ are the eigenvalues of the total angular momentum.

It is advantageous to operate with $\mathcal{P}_L$ on expression (7), which is an expansion in a basis consisting of products of single-particle eigenstates with good angular momenta l_i. Indeed in this case the projection operator acts as a Kronecker delta: from the unrestricted sum (7), it picks up only those terms having a given total angular momentum L. As a result, after taking into consideration the specific electron locations (2) associated with the $(0,N)$ WM, one derives [28] the following symmetry-preserving, many-body correlated wave functions (within a proportionality constant),

$$\Phi^N_L = \sum_{0\le l_1<l_2<\cdots<l_N}^{l_1+\cdots+l_N=L} \left(\prod_{i=1}^{N} l_i!\right)^{-1} \times \left(\prod_{1\le i<j\le N} \sin\left[\frac{\pi}{N}(l_i - l_j)\right]\right) \times D(l_1,l_2,...,l_N) \exp(-\sum_{i=1}^{N} z_i z_i^*/2) \ . \tag{9}$$

In deriving (9), we took into account that for each determinant $D(l_1,l_2,...,l_N)$ in the unrestricted expansion (7) there are $N! - 1$ other determinants generated from it through a permutation of the indices $\{l_1,l_2,...,l_N\}$; these determinants are equal to the original one or differ from it by a sign only. In the case of an $(1,N-1)$ WM, the corresponding correlated wave functions are given by,

$$\Phi'^N_L = \sum_{0\le l_2<l_3<\cdots<l_N}^{l_2+\cdots+l_N=L} \left(\prod_{i=2}^{N} l_i!\right)^{-1} \times \left(\prod_{2\le i<j\le N} \sin\left[\frac{\pi}{N-1}(l_i - l_j)\right]\right) \times D(0,l_2,...,l_N) \exp(-\sum_{i=1}^{N} z_i z_i^*/2) \ . \tag{10}$$

We call the correlated wave functions [Eq. (9) and Eq. (10)] the electron-molecule wave functions (EMWF's). We stress that the EMWF's have good total angular momenta, unlike the UHF determinant from which they were projected out. The projection operator (8) acts on a single UHF determinant, but yields a whole rotational band of the WM. The states in this band are those with the lowest energy for a given angular momentum L, and in addition they are *purely* rotational, i.e., they carry no other internal excitations; in analogy with the customary terminology from the spectroscopy of rotating nuclei [26,29], we designate this band as the "yrast band".

Furthermore, if instead of electrons the displaced Gaussians (1) describe *bosonic* particles forming a molecule, the corresponding [18] many-body correlated wave functions will be given by expressions similar to Eq. (9) and Eq. (10), but with the following two important differences: (I) The product of sine functions will be replaced by a sum over cosines, and (II) The determinants $D(l_1,l_2,...,l_N)$ will be replaced by permanents [30] $P(l_1,l_2,...,l_N) \equiv \mathrm{perm}[z_1^{l_1}, z_2^{l_2}, ..., z_N^{l_N}]$.

Among the properties of the EMWF's specified by Eq. (9) and Eq. (10), we mention the following:

1) The EMWF's lie entirely within the Hilbert subspace spanned by the lowest Landau level and, after expanding the determinants [28], they can be written in the form (within a proportionality constant),

$$\Phi_L^N[z] = P_L^N[z] \exp(-\sum_{i=1}^{N} z_i z_i^*/2) \ , \qquad (11)$$

where the $P_L^N[z]$'s are order-L homogeneous polynomials of the z_i's.

2) The polynomials $P_L^N[z]$ are divisible by

$$P_V^N[z] = \prod_{1\le i<j\le N} (z_i - z_j) \ , \qquad (12)$$

namely $P_L^N[z] = P_V^N[z] Q_L^N[z]$. This is a consequence of the antisymmetry of $\Phi_L^N[z]$. $P_V^N[z]$ is the Vandermonde determinant $D(0, 1, ..., N)$. For the case of the lowest allowed angular momentum $L_0 = N(N-1)/2$ (see below), one has $P_{L_0}^N[z] = P_V^N[z]$, a property that is shared with the Jastrow-Laughlin [2] and composite-fermion [3] trial wave functions.

3) Upon the introduction of the Jacobi coordinates, the center-of-mass separates from the internal variables in complete analogy with the exact solution.

4) The coefficients of the determinants [i.e., products of sine functions, see Eq. (9 and Eq. (10)] dictate that the EMWF's are nonzero only for special values of the total angular momentum L given by,

$$L = N(N-1)/2 + Nk, \ \ k = 0, 1, 2, 3, ... \ , \qquad (13)$$

for the $(0, N)$ configuration, and

$$L = N(N-1)/2 + (N-1)k, \ \ k = 0, 1, 2, 3, ... \ , \qquad (14)$$

for the $(1, N-1)$ one. The minimum angular momentum $L_0 = N(N-1)/2$ is determined by the fact that the D determinants [see Eq. (9) and Eq. (10)] vanish if any two of the single-particle angular momenta l_i and l_j are equal. In plots of the energy vs. the angular momenta, derived from exact-diagonalization studies [5–10], it has been found that the special L values given by Eq. (13) and Eq. (14) exhibit prominent cusps reflecting enhanced stability; as a result these L values are often referred to as "magic angular momenta". We stress that the angular momenta associated with the EMWF's correspond precisely to the magic L's of the exact-diagonalization studies [31]. In the thermodynamic limit [2,5], one can relate the total L to a fractional filling through the relation $\nu = N(N-1)/(2L)$, and thus the EMWF angular momenta (13) and (14) correspond to all the fractional filling factors associated with the FQHE, including the even-denominator ones, i.e., ν = 1, 3/5, 3/7, 5/7, 2/3, 1/2, 1/3, etc...

5) For the case of two electrons ($N = 2$), the EMWF's reduce to the Jastrow-Laughlin form, namely

$$P_L^2[z] = \prod_{1\le i<j\le N} (z_i - z_j)^L \ , \qquad (15)$$

where L = 1, 3, 5, ... However, this is the only case for which there is coincidence between the EMWF's and the JL wave functions. For higher numbers of electrons, N, the EMWF polynomials $P_L^N[z]$ (apart from the lowest-order Vandermonde $P_{L_0}^N[z]$ ones) are quite different from the corresponding JL or composite-fermion polynomials. In particular, the familiar factor $\prod_{1\le i<j\le N}(z_i - z_j)^{2p}$, with p an integer [3,4], (which reflects multiple zeroes) does not appear in the EMWF's (see, e.g., Table I which contrasts the $Q_9^3[z]$ polynomials corresponding to the EMWF's and JL functions).

TABLE I. The $Q_9^3[z]$ polynomial associated with the EMWF's and the JL functions (The $Q_L^N[z]$ polynomials are of order $L - L_0$).

EMWF	$(z_1^3 - 3z_1^2 z_2 + z_2^3 + 6z_1 z_2 z_3 - 3z_2^2 z_3 - 3z_1 z_3^2 + z_3^3)$ $\times(z_1^3 - 3z_1 z_2^2 + z_2^3 + 6z_1 z_2 z_3 - 3z_1^2 z_3 - 3z_2 z_3^2 + z_3^3)$
JL	$(z_1 - z_2)^2 (z_1 - z_3)^2 (z_2 - z_3)^2$

6) For the case of three electrons ($N = 3$), after transforming to the Jacobi coordinates $\bar{z} = (z_1 + z_2 + z_3)/3$, $z_a = (2/3)^{1/2}((z_1 + z_2)/2 - z_3)$, $z_b = (z_1 - z_2)/\sqrt{2}$ (and dropping the center-of-mass exponential factor), the EMWF's can be written as (again within a proportionality constant),

$$\Phi_L^3[z_a, z_b] = [(z_a + \imath z_b)^L - (z_a - \imath z_b)^L] \times \exp[(-1/2)(z_a z_a^* + z_b z_b^*)] \ , \qquad (16)$$

with $L = 3m$, m = 1, 2, 3, 4, ... being the total angular momentum. Again the wave functions $\Phi_L^3[z_a, z_b]$ are very different from the three-electron JL ones; e.g., they are nonvanishing for even m values, unlike the three-electron JL functions. However, the $\Phi_L^3[z_a, z_b]$'s coincide with the functions $|m, 0\rangle$ derived in Ref. [1]. We notice that, although it was found [1,32] that these wave functions exhibited behavior expected of fractional quantum Hall ground states, the generalization of them to a higher number of electrons did not follow.

Several publications [4,6,33] have applied the composite fermion picture (the JL functions are a special case of the CF's) to single QD's in strong magnetic fields. In particular, it has been shown [4] that CF wave functions can be constructed with angular momenta coinciding with the magic ones. However, it has also been found [9] that several discrepancies exist, i.e., some of the larger magic angular momenta are not reproduced by the CF picture. As a consequence of the above, the REM description with the EMWF's derived here offers a natural alternative for interpreting the physics of electrons in QD's in high magnetic fields. This proposition is further supported by inspection of the overlaps between the EMWF's and the exact many-body eigenstates, and their comparison with the corresponding overlaps for the JL states; see Table II, where in some instances (i.e., $N = 4$, $L = 10$ and 14) we list energies of the EM, CF, and exact states instead of the overlaps. Indeed the agreement between the EM

TABLE II. Overlaps, $\langle\phi_L^N|\psi_L^N\rangle/(\langle\phi_L^N|\phi_L^N\rangle\langle\psi_L^N|\psi_L^N\rangle)^{1/2}$, of EMWF's ($\phi$'s) and JL functions ($\phi$'s) with the corresponding exact eigenstates (ψ's) for various values of the angular momenta L. Recall that the angular momenta for the JL functions are $L_{JL} = N(N-1)m/2$, with $m > 0$ being an odd integer. Bottom: Energies of EMWF's compared to CF and exact-diagonalization results. Energies in units of $e^2/\kappa l_B$, (κ is the dielectric constant).

OVERLAPS	L	EMWF	JL	
N=3	9	0.98347	0.99946[a]	
	15	0.99473	0.99468[a]	
	21	0.99674	0.99476[a]	
	27	0.99758	0.99573[a]	
	33	0.99807	0.99652[a]	
	39	0.99839	0.99708[a]	
N=4	18	0.92937	0.97880	
	30	0.96742	0.94749	
	42	0.97366	0.95561	
	54	0.97623	0.96815	
ENERGIES	L	EMWF	CF	EXACT
N=4	10	1.78510	1.78537[b]	1.78509
	14	1.50955	1.50222[b]	1.50066

[a]From Ref. [2].
[b]From Table V of Ref. [33].

states and the exact ones is of comparable quality as in the case of the CF and JL wave functions.

In summary, we have developed a new class of analytic and parameter-free, strongly correlated wave functions of simple functional form, which accurately describe the physics of electrons in QD's under high magnetic fields. The thematic basis of our approach is built upon the intuitive picture of collectively rotating electron molecules, and the synthesis of the many-body EMWF's involves breaking of the circular symmetry at the UHF level with subsequent restoration of this symmetry via a projection technique. While we focus here on the strong magnetic-field regime, we note that the REM picture unifies the treatment of strongly correlated states of electrons in QD's over the whole magnetic-field range [12,22,26]. We also remark that our analysis, aimed here mainly at treating finite electron systems (i.e., QD's) with an arbitrary number of electrons, points to the remarkable conclusion that the observed FQHE hierarchy of filling factors may be viewed as an experimental signature of the yrast band (see above) of the REM.

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